2-Ethoxyethyl methyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, 2-ethoxyethyl methyl ester
Inchi: InChI=1S/C13H16O5/c1-3-17-8-9-18-13(15)11-7-5-4-6-10(11)12(14)16-2/h4-7H,3,8-9H2
InchiKey: MKOHYHMTTKVINI-UHFFFAOYSA-N
Formula: C13H16O5
SMILES: CCOCCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]: 252.26

Physical Properties

Property code	Value	Unit	Source
gf	-411.48	kJ/mol	Joback Method
hf	-708.41	kJ/mol	Joback Method
hfus	29.84	kJ/mol	Joback Method
hvap	68.19	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.666		Crippen Method
mcvol	191.020	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	703.50	K	Joback Method
tc	910.34	K	Joback Method
tf	441.76	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.53	J/mol×K	703.50	Joback Method
cpg	573.00	J/mol×K	875.86	Joback Method
cpg	562.86	J/mol×K	841.39	Joback Method
cpg	551.84	J/mol×K	806.92	Joback Method
cpg	539.94	J/mol×K	772.45	Joback Method
cpg	527.16	J/mol×K	737.97	Joback Method
cpg	582.24	J/mol×K	910.34	Joback Method

dvisc	0.0001039	Pa×s	703.50	Joback Method
dvisc	0.0001299	Pa×s	659.88	Joback Method
dvisc	0.0001676	Pa×s	616.25	Joback Method
dvisc	0.0002248	Pa×s	572.63	Joback Method
dvisc	0.0003164	Pa×s	529.01	Joback Method
dvisc	0.0004738	Pa×s	485.38	Joback Method
dvisc	0.0007681	Pa×s	441.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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